3D Modeling and Simulation of Rechargeable Zinc-Air cells

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In the field of zinc-air batteries, most of the research has an experimental character. We contribute to this topic and support experimentalists with electrochemical models and numerical simulations. Experiments have a long preparation time, work only under certain environmental conditions, or take long to complete. The setup or manufacturing process can also be expensive. In those cases it is favorable to carry out simulations and screen a wide range of parameters, cost and time efficiently. Those parameters are modifications of the geometry, the electrode materials, or the electrolyte [1]. Simulations cannot stand without measurements, but a computational study can significantly improve research and production processes. Most models of zinc-air batteries describe the cell dynamics along one dimension [2,3]. They capture the transport of the concentrations, calculate a consistent electric potential, and regard the temporal changes of the different phases. In some cases, the effect of convection is considered. The models couple the transport equations with the cell reactions. In one dimension, they predict the cell voltage of zinc-air batteries [2]. However, they are not sufficient to describe the local effects of inhomogeneities, which have been measured by [4,5]. Their tomographies show that zinc-air cells have an irregular anode structure and a non-uniform zinc utilization.
In this work, we use a local volume averaging method [6] to transform the thermodynamically consistent bulk equations [7] of highly porous materials to a macroscopic domain. We describe the fluid convection, by a multi-component incompressibility constraint, applied on a concentrated aqueous electrolyte. Our model describes the effects of nucleation, as well as electrolyte carbonation. We make use of three dimensional simulations to understand the intimate correlation between electrode structure, electrolyte composition, and multi-phase coexistence. The electrolyte constituents are water, potassium, hydroxide, zincate, carbonate and dissolved oxygen. We also incorporate passivation effects and consider shape changes of the electrodes.

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